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NETL Report Series Assesses Primary Sources of U.S. Electricity

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Nanostructured Copper Catalysts Show Promise for CO₂ Reuse Applications

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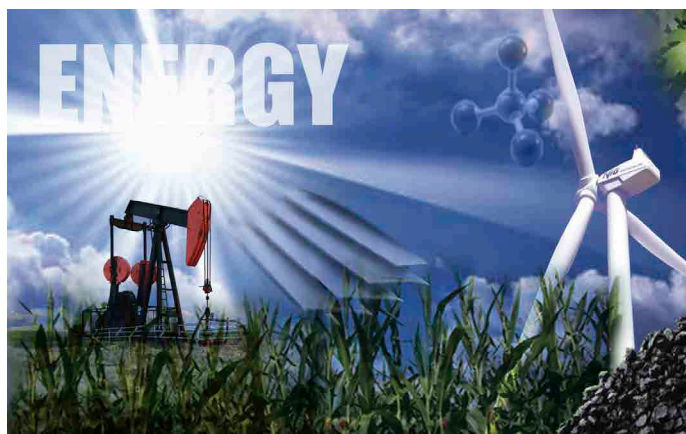
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Cover image: Illustration shows a transparent close-up view for a distillation column in which the animation of the flow rates of the vapor and liquid up and down the column, respectively, are tied to real-time process variables in the dynamic simulator.

netlognews

newlognews is a quarterly newsletter that highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.



NETL Report Series Assesses the Current Role, Life Cycle Environmental Footprint, and Cost for Primary Sources of U.S. Electricity

—The authors of these reports examined the resource base, growth, environmental profile, cost profile, barriers, implementation risks, and expert opinion from stakeholders in academia, government, and private industry for the following power technologies:

- [Pulverized coal and biomass co-firing](#)
- [Natural gas](#)
- [Nuclear](#)
- [Hydropower](#)
- [Wind](#)
- [Geothermal](#)
- [Solar thermal](#)

In a series of seven reports, the analysts employ a consistent modeling approach and framework in assessing the breadth and depth of available knowledge regarding each technology's current role in providing electricity to the nation. The profile of each analysis is based on a life-cycle analysis that accounts for a list of metrics, including availability, cost, and the environment, as well as other issues.

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Illustration shows a transparent view for a distillation column in an IGCC power plant.

IGCC Immersive Training System Deploys at NETL AVESTAR™ Center

—NETL's Advanced Virtual Energy Simulation Training and Research (AVESTAR) team completed the successful deployment and site acceptance testing of a first-of-a-kind 3D virtual immersive training system (ITS) for a commercial-scale integrated gasification combined cycle (IGCC) power plant with carbon capture. The 3D virtual ITS was developed for real-time interactive use with the high-fidelity IGCC dynamic simulator available at the [AVESTAR Center](#). When combined with AVESTAR's state-of-the-art, real-time, high-fidelity IGCC dynamic simulator, the innovative virtual reality technology provides engineers, operators, researchers, and students with hands-on operations, control, and safety experience in a highly realistic, integrated, IGCC plant and control room environment.

Wearing wireless 3D video glasses or a personal 3D viewer head-mounted display, ITS users can interact with IGCC plant equipment items (e.g., valves, pumps, gasifiers, turbines), activate transparent views (e.g., liquid level in a tank), display pop-up trends (e.g., gas turbine combustor temperature over time), and experience equipment sound effects (e.g., pump start/stop), malfunctions (e.g., leaks, fires), and visual training scenarios (e.g., CO₂ absorber column operation).

Using the ITS, IGCC field operators can coordinate activities with control room operators. Immersed in the virtual environment, field operators can move and interact as if they were in the real plant. The environment is fully interactive with

the dynamic simulation models, so actions taken by a field operator will have an impact on the process and actions performed in the control room will change the information visible to the field operator. As a result, field and control room operators are trained to coordinate their activities and perform collaboratively as a team. Additional benefits include training for safety-critical tasks, rare abnormal situations, and emergency shutdowns.

Deployed at the AVESTAR Center in July 2012, the IGCC 3D virtual ITS was developed by NETL in collaboration with Invensys Operations Management, West Virginia University, and Fossil Consulting Services. The same team developed the IGCC dynamic simulator in collaboration with Enginomix, the Electric Power Research Institute (EPRI), and five EPRI CoalFleet industry partners, including American Electric Power, BP Alternative Energy, Doosan, Great River Energy, and Southern Company. The IGCC dynamic simulator was deployed at the AVESTAR Center in March 2011 and recently won a 2012 Excellence in Technology Transfer Award from the Federal Laboratory Consortium Mid-Atlantic Region.

Contact: [Stephen E. Zitney](#), 304-285-1379

Computational Modeling Software Applied to a Discrete Chemistry Model

—For the first time, the NETL Carbonaceous Chemistry for Computational Modeling (C3M) software has been applied to a discrete chemistry model in Multiphase Flow with Interphase eXchanges (otherwise known as MFIX)—Discrete Element Method. While researchers have for some time used the C3M kinetic output for continuum and discrete phase models, computations have largely been volume-averaged based. Now, researchers can gather large amounts of information on individual particle histories not previously possible with the continuum, volume-averaged chemistry models, allowing the tracking of temperature, size, reaction rates, composition, energy transfer, and position for every particle in a model with C3M kinetics applied. The new capability will allow researchers to refine chemical models and improve the correlation of kinetic data to experimental conditions.

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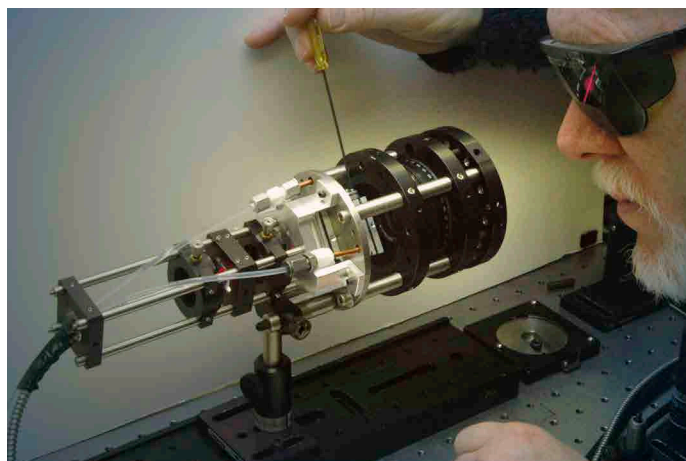
A rendering of a typical sensor with the outside shielding partially removed, displaying the sensor electrodes, data acquisition system, and a laptop (L to R).

Novel Sensor Provides Insight to Flow of Solids

—Our researchers are applying Electrical Capacitance Volume Tomography (ECVT), developed by Tech4Imaging, to quantify solids concentration and bubble dynamics in a fluidized bed. The ECVT sensors allow for a non-intrusive, three-dimensional measurement of solids concentrations in gas-solid, gas-liquid, and liquid-solid multiphase flow systems. Certain behaviors of fluidized beds, such as solids concentration distribution, bubble diameter, bubbling frequency, bubble coalescence, and break up, can be visualized using this technology.

The significant insight gained from quantitative ECVT data will lead to methods for better gas-solid mixing and lower gas bypassing, thereby increasing the performance of reacting systems based on fluidized beds such as carbon capture processes, chemical looping combustion, and gasification. The quantitative data will also support continued development and validation of multiphase flow computational fluid dynamic models used to design of various chemical processes, allowing the prediction of performance before a unit is built. Much industrial and academic interest has been expressed for the technology and for potential collaborations.

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NETL scientist Steven Woodruff makes lab-bench adjustments on the prototype laser spark plug.

NETL Laser Spark Plug Featured in Photonics Spectra

—An article titled, “Laser Car Ignition Dream Sparks Multiple Approaches,” by Laura Marshall was featured in the September issue of *Photonics Spectra*. This story highlights the laser spark plug technology developed at NETL by Dr. Steven Woodruff and Dr. Dustin McIntyre. The article looks at the application of laser spark plugs to automobiles, but draws heavily on the natural gas fueled engine studies done at NETL.

The laser spark plug project is currently seeking new funding through collaboration with the West Virginia University's Department of Mechanical and Aerospace Engineering and is also being applied to sensors with Laser Induced Breakdown Spectroscopy, LIBS.

Contact: [Steven Woodruff](#), 304-285-4175

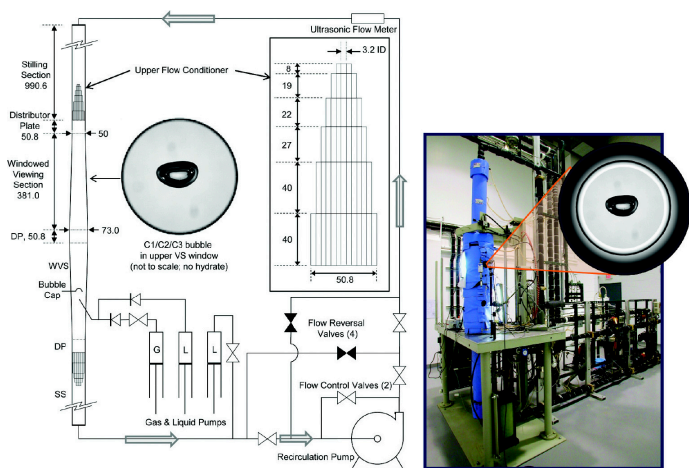


Illustration showing NETL's High-Pressure Water Tunnel Facility.

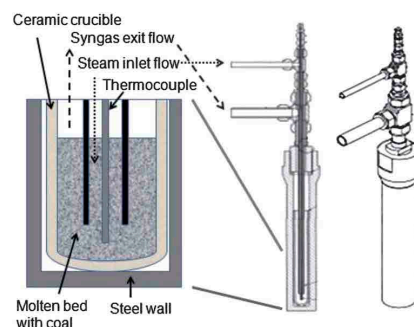
Impacts of Gas Hydrates on Deepwater Hydrocarbon Production Operations

NETL researchers, in conjunction with researchers from Shell International Exploration and Production, Inc., Texas A&M University, Southwest Research Institute, and the Colorado School of Mines, have published a peer-reviewed paper entitled, "Hydrates in the Ocean Beneath, Around, and Above Production Equipment," (*Energy & Fuels*, 2012, 26, 4167-4176).

The NETL contribution to this research was performed in its unique High-Pressure Water Tunnel Facility and involved a study of hydrate formation on single bubbles of a gas mixture consisting of methane, ethane, and propane in proportions thermodynamically similar to gas released from the 2010 Macondo well blowout in the Gulf of Mexico.

This work helped highlight the role of dissolved gas concentration on the hydrate formation process and the propensity of hydrates to form only in areas where dissolved gas concentrations in seawater exceed those observed in nature by several orders of magnitude. Such areas can occur in and around production equipment in areas that trap or limit the natural flow of seawater exposed to a source of hydrocarbon gas. Overall, the paper provides important guidelines for managing and mitigating unwanted hydrate occurrences that could disrupt normal deepwater operations.

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Coal Gasification Demonstrated with in situ Capture of CO₂ and Hydrogen Sulfide

NETL has developed a molten catalytic process for converting coal into a synthesis gas consisting of roughly 20% methane and 80% hydrogen using alkali hydroxides as both gasification catalysts and in situ CO₂ and hydrogen sulfide (H₂S) capture agents. This hydrogen- and methane-rich output from the gasifier could be sent to gas turbines or solid oxide fuel cells in order to generate electricity with CO₂ emissions significantly less than 1.0 lbs of CO₂ per kWh of electricity.

A patent application on this topic has been submitted and a paper entitled "Molten Catalytic Coal Gasification With In Situ Carbon and Sulphur Capture" was published by the Royal Society of Chemistry's journal *Energy & Environment Science*.

Baseline studies were conducted using no catalyst, weak capture agents (calcium silicate), and a strong in situ capture agent for acid gases (calcium oxide-CaO). Parametric studies were conducted to understand the effects of temperature, pressure, catalyst composition, steam flow rate and the ratio of coal to alkali hydroxide on the performance of the molten catalytic gasifier in terms of kinetics and syngas composition.

To measure the amount and the rate of coal conversion, the researchers developed a method for quantifying the coal conversion related to the chemical oxygen demand remaining in the coal. This method was necessary because the capture reactions and the water condenser before the mass spectrometer make a real-time elemental balance impossible.

For many different reforming, gasification, and combustion experiments, measuring the change in the chemical oxygen demand of coal/fuel can be a more useful definition of coal/fuel utilization than measuring the change in the weight of the coal/fuel or measuring the change in carbon content of the coal/fuel.

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Dr. Alexandra Hakala in the laboratory at the National Energy Technology Laboratory.

Researcher Receives Outstanding Technical Achievement Award

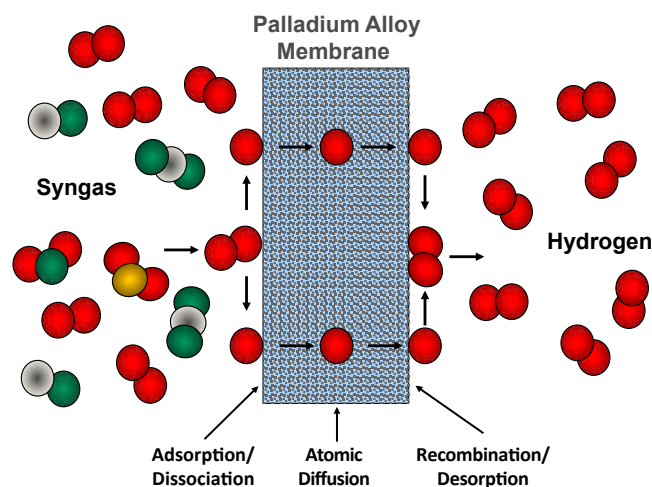
NETL's Dr. Alexandra Hakala has been honored with the Great Minds in STEM™ Hispanic Engineer National Achievement Awards Corporation (HENAAC) award for Outstanding Technical Achievement. Great Minds in STEM™ considers nominees for its awards to be "top role models" in science, technology, engineering, and math (STEM) fields and uses the HENAAC awards to "promote and highlight Hispanic engineers and scientists."

Dr. Hakala serves as the technical coordinator for shale gas research, managing multiple projects within NETL's Office of Research and Development. She also leads two research teams while performing her own research.

Dr. Hakala communicates her research to a wide audience through her published papers and national and international conference presentations, making a significant contribution to energy research. Her innovation and inspiration help guide young scientists as they pursue graduate and post-graduate degrees. She ensures that her interns complete their theses and provides career advice.

Dr. Hakala will receive her award at the 24th Annual HENAAC Conference, *STEM, Excellence, and the Pursuit of Innovation*, on October 12, 2012. Full story here.

Contact: [Alexandra Hakala](#), 412-386-5487



Schematic of hydrogen separation from synthesis gas in coal gasification.

Researchers Improve Hydrogen Separation in Coal Gasification

To produce high purity hydrogen fuel from coal, hydrogen gas has to be extracted from synthesis gas (syngas), a product of coal gasification. Using gas separation membranes is one way to achieve this goal. Although a variety of hydrogen separation membrane materials exist today, none of them are shown to be suitable for employment in contaminant-laden syngas at elevated temperatures.

Surface poisoning and corrosion are shown to be the most significant degradation mechanisms acting on the hydrogen membrane materials at elevated temperatures in synthesis gas derived from coal. Among other metallic dense membrane materials, copper-palladium alloys have demonstrated promise for being resistant against these degradation mechanisms.

NETL materials researchers discovered that the addition of magnesium extends the elevated-temperature structural stability of materials showing promise for separating hydrogen from coal-derived syngas. The copper-palladium-magnesium formulation maintains its more open body-centered cubic crystal structure, which is associated with high hydrogen flux, at significantly higher temperature than copper-palladium alloys.

The researchers predicted magnesium would have this stabilizing potential from first principles density functional

theory calculations. A microstructural characterization of the newly developed hydrogen separation membrane alloy has been published in Elsevier's *Journal of Alloys and Compounds*, Vol. 528 (2012), pp. 10-15.

This research was performed in support of NETL's Fuels Program of the Strategic Center for Coal.

Contacts: [Ömer Doğan](#), 541-967-5858 and [Michael Gao](#), 541-967-5869

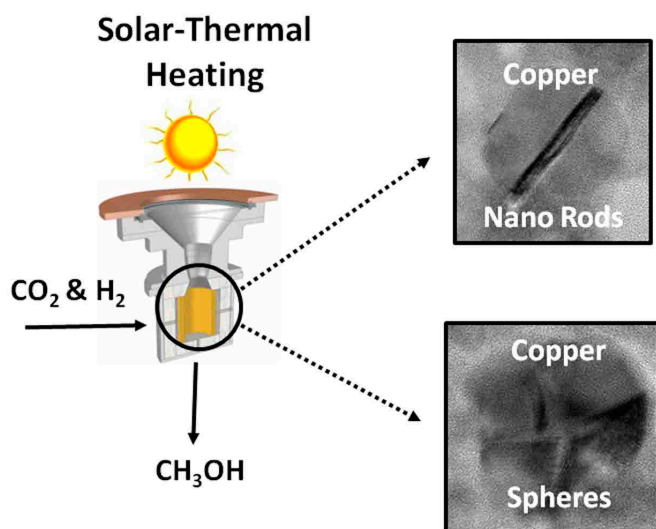
to methanol. Since surface atoms are key for dictating this reaction, developing insight into this process would enable scientists and engineers to improve catalytic performance.

A team of NETL scientists has been able to shed new light on this problem by utilizing nanostructured copper catalysts on metal oxide supports such as zinc oxide. Copper is commonly used in electrical wiring, and zinc oxide is a component of over-the-counter creams, lotions, and sunscreens, thus illustrating how energy technologies can be enhanced by common household items. These everyday items start to display extraordinary properties when shrunk in size to nanometer size scales where the copper has an enhanced reactivity due to its increased surface-to-volume ratio.

The scientists were able to systematically control the nanometer scale size of the copper particles, as well as their dispersion and interaction with the zinc oxide support. Their data shows that catalysts composed of small copper particles are far more reactive than larger ones, presumably due to their increased surface area. The team was also able to show that a synergistic interaction between the copper particles and zinc oxide support contributes to the reaction.

Their results helped resolve a long-standing debate in the scientific literature regarding the role of copper particle size and interactions with support oxides on catalytic performance. These findings indicate that industrial catalysts should focus on utilizing nanometer sized copper particles on oxide supports for improving the reactive throughput. The results of this research have been published in the highly regarded *ACS Catalysis*, Vol 2, pg. 1667-1676, 2012.

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Schematic diagram showing how nanostructured copper catalysts can be incorporated into a carbon friendly CO₂ to methanol reactor using solar energy to heat the catalyst bed.

Nanostructured Copper Catalysts Show Promise for CO₂ Reuse

Applications—The catalytic conversion of CO₂ to methanol (CH₃OH) has the potential to help reduce CO₂ emissions and create a revenue-generating product stream with demand in both the industrial and transportation sectors. Despite a yearly methanol market of almost 110 billion pounds (50 megatonnes), the preparation of highly active catalysts in industry is still more of an art form than a science. In simplistic terms, this means industrial engineers understand how to make catalysts which work well, but still have not been able to develop a complete understanding of how the atoms on the surface of the catalysts facilitate the conversion of CO₂

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10.	Zhi, Mingjia; Lee, Shiwoo; Miller, Nicholas; et al. May 2012. An Intermediate-Temperature Solid Oxide Fuel Cell with Electrospun Nanofiber Cathode, <i>Energy & Environmental Science</i> , 5 (5) 7066-7071.
11.	Minsley, Burke J.; Smith, Bruce D.; Hammack, Richard; et al. May 2012. Calibration and Filtering Strategies for Frequency Domain Electromagnetic Data, <i>J. Applied Geophysics</i> , 80, 56-66.
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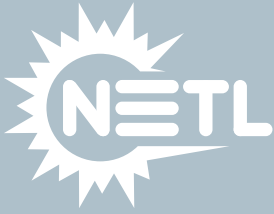
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2.	Pyrochlore Catalysts for Hydrocarbon Fuel Reforming, David A. Berry, Dushyant Shekhawat; Daniel Haynes; Mark Smith, James Spivey, Patent number 8,241,600 , issued August 14, 2012.





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